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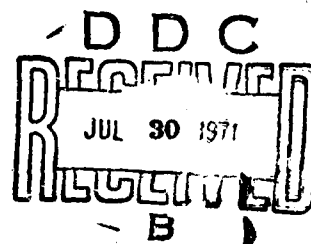
Computer Program for Determining Optical Constants of a Film on an Opaque Substrate

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FOREWORD

The development and continued improvement of target-acquisition and missile-guidance systems for Fleet use are areas of special interest to the Navy. In support of these interests, the Naval Weapons Center (NWC) is conducting research projects in the fields of infrared and ultraviolet detection, solid state physics, and optics. To provide better optical target-acquisition and guidance systems, improvements are required either in systems sensitivity or in operating wavelength range. NWC's research efforts have been directed toward the production of improved detectors and optical elements.

One of the principal efforts in the optics field has been the study of corrosion films on metal surfaces. Since silver has the highest reflectance of any metal in the visible and infrared spectrum, the tarnish layer that forms on silver surfaces is of special concern. During studies conducted at NWC to investigate the growth of silver sulfide tarnish films on silver, it became necessary to obtain the optical constants of the tarnish films. However, since the films could not be removed from the substrate, conventional methods used to determine these constants were not applicable. Consequently, a computer program was developed to determine the optical constants of films on opaque substrates by using input data obtained from normal incidence reflectance measurements on two films of different thicknesses. This computer program is described in the included reprint of an article published in *Applied Optics*, Vol. 8, No. 11 (November 1969), pp. 2366-68.

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Computer Program for Determining Optical Constants of a Film on an Opaque Substrate

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In the course of studying the growth of silver sulfide tarnish films on silver,¹⁻⁴ we needed to know their optical constants, n - jk . The films were under 100-Å thick and could not be removed from the silver, so that we were unable to use the method of determining n and k from the measured reflectance R , transmittance T , and film thickness t .⁵ We thus decided to try to obtain the optical constants from normal incidence reflectance measurements on two silver sulfide films of different thicknesses on silver where the sulfide thicknesses were measured ellipsometrically.² This involved an addition to our multilayer film computer program which will be described in this letter.

The basic multilayer film program⁶ calculates reflectance, transmittance, and phase change on reflection of a substrate covered with one or more films of known thickness and optical constants, when the optical constants of the substrate are also supplied. This program was previously modified to obtain n and k for a film given the refractive index of the (transparent) substrate,

film thickness, normal incidence front surface reflectance, and transmittance of the film on the substrate.⁶ The program described in this letter is independent of the R , T , and t modification, although it uses some of the same logic and iterative techniques.

The addition to the multilayer film program which is required for the new calculational method is shown in the flow diagram in Fig. 1. The reflectance R_c of the opaque substrate is first calculated using assumed optical constants for the substrate material. (For silver, the solution is not very sensitive to the values chosen.) Trial values of n and k for the film are then taken along with the film thickness t_1 , and the reflectance R_{1c} is calculated for the film on the opaque substrate. R_{1c} is subtracted from R_c and a quantity called ΔR_{1c} is obtained. A second quantity, ΔR_{2c} , for a film of thickness t_2 is obtained in an analogous manner. These ΔR 's should be directly comparable with the measured quantities ΔR_1 and ΔR_2 obtained by subtracting the measured reflectance of a film-covered opaque substrate from the reflectance of the film-free substrate.

The major portion of the new program consists of changing n and k for the films in such a way that $\Delta R_{1c} = \Delta R_1$ and $\Delta R_{2c} = \Delta R_2$. Since there are two measured quantities, ΔR_1 and ΔR_2 , and two unknowns, n and k for the films, in principle a unique solution should exist if both films have the same optical constants. (In practice there are experimental difficulties which prevent

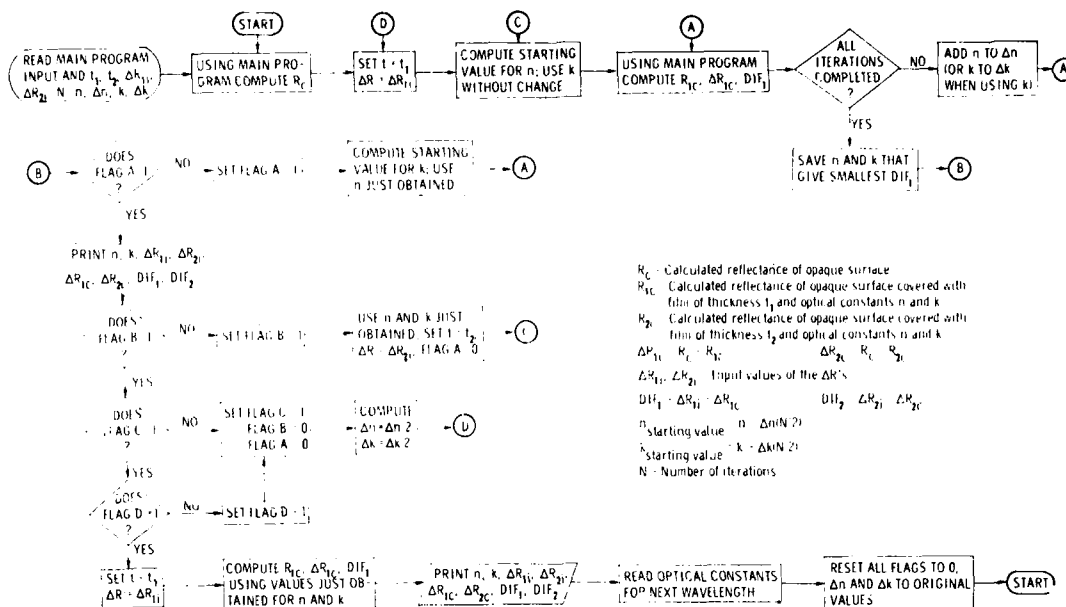


Fig. 1. Flow diagram for addition to multi-layer film program which determines optical constants of a film on an opaque substrate.

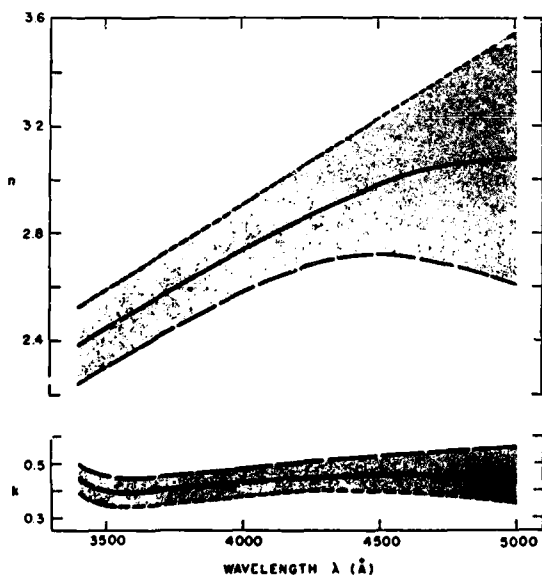


Fig. 2. Range of n and k values which give ΔR 's within 0.001 of the input values for films of thicknesses 22.5 Å and 38 Å, respectively. The short-dashed n curve goes with the short-dashed k curve and the long-dashed n and k curves similarly go together.

unique solutions from being obtained; these will be discussed later.) The detailed manner in which the search routine proceeds can be summarized as follows. From the trial values of n and k for the films, a range of values of n is selected centering on the trial n value. With k held fixed, ΔR_{1c} is calculated for all the n values selected, and the n saved which gives a ΔR_{1c} closest to ΔR_{1i} (i.e., smallest DIF_1 —see Fig. 1). Using this n , the trial value of k is now varied over a selected range and the k giving the smallest DIF_1 is retained. Using this new pair of n and k values, the program shifts to the second film of thickness t_2 and repeats the process, obtaining a different pair of n and k values which yield the smallest DIF_2 . The preceding process is called cycle I. Cycle II consists of a repeat of cycle I starting with the just-determined n and k , only letting the allowed ranges of values of n and k be exactly half the allowed ranges for cycle I. Cycle III is a repeat of cycle II with the allowed ranges again cut in half.

If the allowed ranges of n 's and k 's are properly chosen, the program should converge on a single pair of values which satisfy the conditions $\Delta R_{1c} = \Delta R_{1i}$ and $\Delta R_{2c} = \Delta R_{2i}$ (i.e., $DIF_1 = DIF_2 = 0$). However, if the range of n 's is too large, ΔR_{1c} can be made equal to ΔR_{1i} by simply changing n (k not required to change). In this situation, when going to ΔR_{2c} , n may change to a different value, still without requiring k to change. In cycles II and III, the major portions of the changes may again be made by n , so that there appear to be two discrete values of n corresponding to film thicknesses t_1 and t_2 . If this situation occurs, the allowed range of n should be made smaller so that k will also have to change. If discrete solutions for n are found for the two films even though k is allowed to change, the two films may actually have different optical constants.

If ΔR_{1i} and ΔR_{2i} are exact and the two films have the same optical constants, the calculated n and k values will be unique. However, if the ΔR 's contain experimental measuring errors, a series of solutions for n and k will be obtained where the range of values will depend on the percentage uncertainty in the ΔR 's. As an example, consider the following problem. For two films of silver sulfide on silver (thicknesses 22.5 Å and 38 Å, respectively) we have measured values of ΔR_1 and ΔR_2 which we will use as inputs. [For the purpose of this problem, the so-called mea-

sured quantities were actually calculated from the thin-film optical constants in Ref 4.] After choosing a set of trial values of n and k for the silver sulfide films and using the computer program, we obtain the values of n and k shown as the solid lines in Fig. 2. However, our measured values, ΔR_{1i} and ΔR_{2i} , are not exact, but each contains a measuring uncertainty of ± 0.001 . To find the upper limit of n values which can be a solution, we choose a value of n larger than that on the solid line and restrict it to a very narrow range of values. We then use the program to find a single k value which gives the smallest DIF_1 and DIF_2 . If these differences are less than 0.001 in absolute value, we have a solution. However, we want the n value where both DIF_1 and DIF_2 are close to 0.001, so a larger n is chosen until one is found where they are. If either DIF_1 or DIF_2 is larger than 0.001, we have chosen our initial n too large and must reduce it. We can similarly find the lower limit of n values using n 's smaller than the numbers on the solid curve. Results of these calculations are shown as the shaded area in Fig. 2. In this figure the short-dashed n curve and the short-dashed k curve are solutions for which the ΔR 's are exactly ± 0.001 different from the original values; the long-dashed n and k curves are also solutions satisfying this requirement. Although these curves are strictly representative only of the particular example of silver sulfide on glass, the generalizations can be drawn. At the long wavelength end of the region, the ΔR 's are small ($\Delta R_{1i} = 0.037$ and $\Delta R_{2i} = 0.072$ at 5000 \AA) so that an error of ± 0.001 creates a large spread in n . In contrast, at 3400 \AA , $\Delta R_{1i} = 0.178$ and $\Delta R_{2i} = 0.303$ so the percentage error in the ΔR 's is smaller and n and k have a smaller spread.

In the preceding discussion we have been assuming that the film was absorbing (i.e., k nonzero). If k is known to be strictly zero, the method can still be used by restricting k to very small values which change the ΔR 's by less than the measuring error. The program will then find the correct n for the films (or try to converge on two different n 's if the two thicknesses have different refractive indices). This procedure was tried for a calculated case of aluminum oxide films on aluminum, and we found that the

correct n values were obtained as long as k was kept small enough. If k was allowed to be larger, the n values were in error, the amount of the error depending on the allowed magnitude of k .

We have also assumed that the film thickness was correctly known and had no error associated with it, not a realistic assumption. The effect of an error in film thickness can easily be determined by changing one or both of the film thicknesses by the amount of the supposed error and by noting what happens to the calculated optical constants. It is not easy to generalize on the effect of a thickness error since it depends strongly on the particular problem. However, as the films become thicker and the two thicknesses become widely different from each other, a constant absolute error in t becomes a smaller percentage error and thus has less effect on the solution. Likewise, the range of solutions for n and k becomes smaller with increasing film thickness and eventually n and k become unique.

In conclusion, we have described a method for obtaining optical constants of a film for the case when the film is on an opaque substrate. The method does not necessarily give unique solutions unless other information about either n or k is supplied. If either n or k is known exactly, unique solutions can be obtained.

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ABSTRACT CARD

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